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Application of near-infrared spectroscopy to wood discrimination

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Abstract This study deals with a new nondestructive discriminant analysis by which wood can be classified on the basis of a combination of near-infrared (NIR) spectroscopy and Mahalanobis' generalized distance. Its accuracy and reasonability were examined for wood samples with various moisture contents ranging from oven-dried to a fully saturated free water state. In a discriminant analysis employing second derivative spectra, each wood group was well distinguished. Mahalanobis' generalized distances between softwoods are relatively independent of analytical pattern, whereas the distances between hardwoods are large for easy classification. There may be two reasons for selecting a wavelength: (1) when the chemical component of wood substance relates to the discriminant analysis; and (2) when the difference in moisture content with wood species relates to them. When we correctly construct the database of NIR spectra, confirming the purpose of the analysis, suitable wood discrimination should be possible.

Key words Near-infrared spectroscopy · Nondestructive measurement · Discriminant analysis · Mahalanobis' generalized distance

Introduction

Near-infrared spectroscopy (NIRS) is a nondestructive analytical method for determining the composition of materi-

als.^{1,2} Diffuse reflectance or an absorption spectrum over 800–2500nm allows clear discrimination of various organic compounds. In the fields of foods, medicines, papers, and so forth, intense interest has been directed toward NIRS because of its accuracy and rapidity. Recently, we examined the nondestructive assessment of moisture and physical conditions in bulky wood by NIRS. The calibration equations for moisture content and orientation of fiber, among other parameters, were determined from a multiterm linear regression analysis with sufficient precision.^{3–5} Many researchers have also reported the application of NIRS to wood science and technology. For example, Thygesen and Lundqvist^{6,7} examined NIR measurements of moisture content in wood under unstable temperature conditions. Hoffmeyer and Pedersen⁸ reported the usefulness of this technique as a nondestructive measurement of the density and strength of Norway spruce. Schimleck et al.⁹ applied NIR spectra to the evaluation of the chemical components of *Eucalyptus* from the viewpoint of an important determinant of pulpwood quality. Applications of NIRS to wood-based material were also reported by Kniest¹⁰ and Niemz et al.¹¹

Thus, NIRS has been generally characterized as a nondestructive quantitative measurement, but there are other options for qualitative analyses based on a mathematical-statistical method, which would be preferable for the wood industry. For example, it is important for timber marketing or warehouse management to discriminate the wood species and its quality correctly before forwarding it to the market. However, a drop in the number of skilled inspectors and the diversification of utilized wood species have resulted in an interruption of such inspections. An effective method for improving these circumstances is therefore required worldwide in regions where unfamiliar wood species are utilized.

Brunner et al.¹³ have already demonstrated the usefulness of Fourier transform (FT)-NIR for the classification of wood species. They employed original NIR spectra (1000–2200nm) of various sawn, cut, or microtomed samples for the principal component analysis, so the physical structure of the sample surface is directly affected on cluster analysis.

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It is desirable to find the key wavelengths over the NIR range (800–2500 nm), which contributes to sample classification with statistical satisfaction. We focused our attention on these problems and now propose a new analytical procedure by which wood discrimination could be performed well under the required sample conditions. NIR spectra of nine wood species with moisture contents ranging from oven-dried to the fully saturated free water state were measured. For these spectroscopic results that included second derivative spectra, the Mahalanobis' generalized distance between each group was calculated to find a suitable analytical pattern that was not affected by the moisture content. Thus, the accuracy and reasonableness of wood discrimination were variously examined.

Concept of Mahalanobis' generalized distance

In qualitative analysis of spectra from an unknown sample, the restricted regions of the spectrum are focused to classify or identify the sample by matching the location and strength of absorbance peaks to those of known substances. By plotting the absorbance readings at one wavelength λ_1 versus the corresponding readings at another wavelength λ_2 , we obtain the results shown in Fig. 1, in which groups of three materials are well separated. This indicates that the spectra of the materials concerned are sufficiently different at these two wavelengths. In general, however, we could not expect to classify a large number of materials using only two wavelengths.

It is possible to classify samples by defining the locations of the various groups in these spaces and assigning a sample to a group if it is "near" that group. In this study we focused on the statistical distance between samples for a mathematical description of the discriminant analysis.¹² A distance measure D_i of i th group is characterized such that the equivalent Euclidean distance is large in those directions in which the group is elongated. The quantity D_i , defining the unit distance vector in multidimensional space, is called Mahalanobis' generalized distance. It can be described by an ellipse (Fig. 1). The distance D_i from point x to the center of group x_i is described by the matrix equation

$$D_i^2 = (X - X_i)' M (X - X_i) \quad (1)$$

where X is the multidimensional vector describing the location of point x , X_i is the multidimensional vector describing the location of the group mean of the i th group, $(X - X_i)'$ is the transposition of the vector $(X - X_i)$, and M is a matrix determining the distance measures of the multidimensional space involved.

In this study, the boundary of a group was defined to be 3 SD away from the group mean. We could then assign a sample within 3 SD of a group to that group unambiguously. Also, if two groups have their group means within 6 SD of each other, the boundaries of the two groups overlap, and we are warned of the possibility of misclassification.

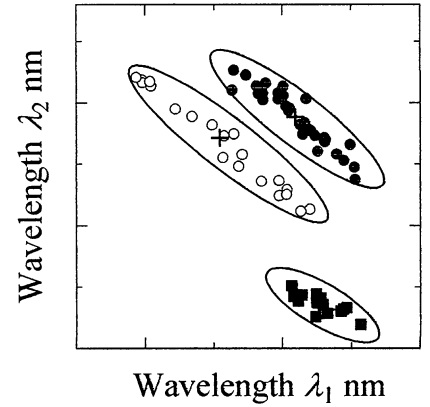


Fig. 1. Typical two-dimensional wavelength space

Table 1. Tested species

Species	Density in oven-dried state (g/cm ³)
<i>Cryptomeria japonica</i> D. Don	0.29
<i>Pseudotsuga menziesii</i> Franco	0.44
<i>Picea sitchensis</i> Carr.	0.57
<i>Tectona grandis</i> Linn.	0.56
<i>Quercus mongolica</i> Fisch var.	0.69
<i>Paulownia tomentosa</i> Steud.	0.24
<i>Quercus gilva</i> Blume	0.66
<i>Fagus crenata</i> Blume	0.68

Material and methods

Samples

Table 1 shows the wood species used for the analysis. The dimensions of the samples were 30 × 30 × 10 mm (sample surface 30 × 30 mm). Each sample, corrected from the same log, was finished by the surfacer. The irradiation surface of the wood coincided with the flat grain or edge grain. The *Cryptomeria* group was composed of a mixture of sapwood and heartwood or sapwood alone. Other groups were composed of only sapwood. We controlled the moisture conditions as follows.

1. The wood samples were humidified ranging from the oven-dried state to the fiber saturation state using desiccators under several relative vapor pressures. There were 48 samples for each wood species: 30 were employed for the data set, and 18 were employed for validation. In this case, each sample had a homogeneous moisture distribution.
2. Wood samples in a fully saturated free water condition were prepared. Each sample was dried indoors [23°C; 45% relative humidity (RH)] for the required time. There were 20 samples for each wood species: 15 were employed for the data set, and 5 were employed for validation. In this case, each sample had an inhomogeneous moisture distribution.

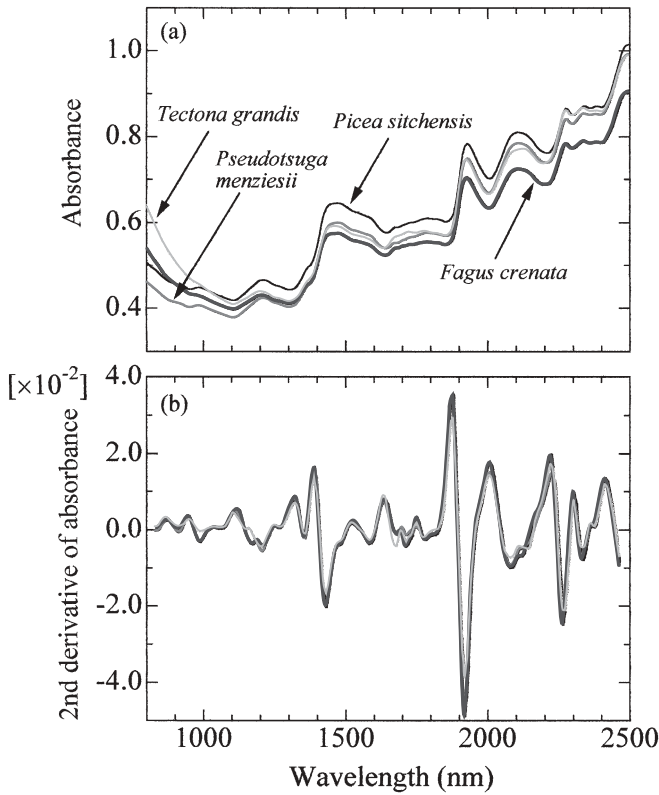


Fig. 2. Near-infrared spectra of various wood species. **a** Original spectra. **b** Second derivative spectra. Moisture content: air-dried condition

Measuring apparatus

The instrument used to measure absorbance was an InfraAlyzer 500 (Bran+Luebbe). The integrating sphere in this system was utilized to collect the diffusely reflected light. The surface of a sample was irradiated perpendicularly with a series of NIR monochromatic lights. The wavelength of the incident light varied from 800 to 2500 nm in steps of 4 nm.

We measured original and second derivative spectra to examine not only the best classification condition but also the reasonableness of the selected wavelength (Fig. 2). These spectra could explain the assignment of an absorption band to a sample. The wavelengths for defining the second or third dimensional space were selected from the whole NIR range (800–2500 nm) or the short-wavelength range of 800–1100 nm, where we observed molecular vibration of the second overtone.¹ These two or three wavelengths were selected for the best classification.

Outline of experiment

The procedures for the discriminant analysis were as follows. The NIR spectra for the samples were measured and were divided into the data set constructing each group and the unknown data for validation. The multidimensional spaces were constructed by selecting some wavelengths, where we discriminated between various materials using

as many wavelengths as necessary to distinguish them. Thereby, the wavelengths were selected mathematically to separate each group as clearly as possible. In these cases it was not necessary to find an expressive relation between the selected wavelengths and the assignment of an absorption band in the NIR spectrum. The distance between point x for the validation sample and point x_i for the group mean of the i th group was calculated, by which the nearest group to be assigned was determined.

Results and discussion

Mahalanobis' generalized distance between wood groups

The Mahalanobis' generalized distances between the various groups were calculated for the data set. These distances in the required discrimination pattern are displayed in Tables 2 and 3, where the best three wavelengths were chosen from the restricted NIR range. In Table 2 the moisture content was in the range from the oven-dried state to the fiber-saturated state. In Table 3 the moisture content was in the range from the air-dried state to the fully saturated free water state. As the distance increases we can easily find the differences for each wood group. According to our definition for such a discriminant analysis, the groups closer than six Mahalanobis' generalized distances overlap, potentially causing misclassification. As shown in Tables 2 and 3, we could not find the best circumstance at which all distances should be more than 6σ . However, we may conclude that every group is almost well separated when the wavelength is selected within the whole NIR range (800–2500 nm) (Table 2a,b or Table 3a,b). In the discriminant analysis, it may be safe to say that we consider the boundary of a group to be 2 SD away from the group mean. According to this definition, all groups in Table 2b could be well separated.

The distances between softwoods are relatively small, independent of the analytical pattern, so it is difficult to grasp the difference in their spectroscopic characteristics. However, improved classification may be expected by increasing the number of selected wavelengths. On the other hand, the distances between hardwoods are large and result in easy classification. Some physical structure and chemical components are directly related to these results. The effect of lignin or extractives on the difference in the NIR spectra of wood may be marked. When we correctly construct the database for the NIR spectra, confirming the purpose of the analysis, automation of the discriminant analysis will be possible.

The sum of the inverse squared distance between all pairs of wood groups S_{isd} was devised to examine synthetically the effect of the moisture condition, the selected wavelength, or the wavelength range on the variation in Mahalanobis' generalized distances.

$$S_{\text{isd}} = \sum \left(\frac{1}{D_i} \right)^2 \quad (2)$$

Table 2. Mahalanobis' generalized distance between wood species using oven-dried to fiber-saturated samples

Sample	<i>Pseudotsuga</i>	<i>Cryptomeria</i>	<i>Cryptomeria</i> S.	<i>Fagus</i>	<i>Quercus m.</i>	<i>Tectona</i>	<i>Paulownia</i>	<i>Quercus g.</i>
(a) Original spectra; NIR range for selecting wavelengths: 800–2500 nm								
<i>Picea</i>	3.21 ^a	8.81	10.91	24.99	18.81	12.52	24.32	18.21
<i>Pseudotsuga</i>		6.41	7.97	24.71	18.01	11.63	22.16	16.14
<i>Cryptomeria</i>			3.27 ^a	20.28	13.17	7.01	15.80	10.10
<i>Cryptomeria</i> S.				22.14	14.85	9.46	15.17	9.92
<i>Fagus</i>					7.36	13.43	15.76	14.71
<i>Quercus m.</i>						6.73	11.49	8.06
<i>Tectona</i>							13.54	8.13
<i>Paulownia</i>								6.64
(b) Second derivative spectra; NIR range for selecting wavelengths: 800–2500 nm								
<i>Picea</i>	4.55 ^a	9.22	11.62	27.53	15.90	5.98	17.39	13.35
<i>Pseudotsuga</i>		5.73 ^a	8.89	30.01	18.81	7.36	15.71	14.33
<i>Cryptomeria</i>			3.48 ^a	29.26	19.23	8.43	10.79	12.54
<i>Cryptomeria</i> S.				27.63	18.54	9.29	7.48	10.89
<i>Fagus</i>					11.76	22.77	23.89	16.81
<i>Quercus m.</i>						11.71	17.71	8.44
<i>Tectona</i>							12.91	7.97
<i>Paulownia</i>								9.37
(c) Original spectra; NIR range for selecting wavelengths: 800–1100 nm								
<i>Picea</i>	1.91 ^a	9.97	8.39	4.29 ^a	8.02	18.16	13.29	11.75
<i>Pseudotsuga</i>		8.07	6.48	2.56 ^a	6.24	16.41	11.37	9.87
<i>Cryptomeria</i>			2.29 ^a	5.94 ^a	3.21 ^a	9.39	3.52 ^a	2.57 ^a
<i>Cryptomeria</i> S.				4.85 ^a	3.72 ^a	11.63	5.16 ^a	4.62 ^a
<i>Fagus</i>					3.85 ^a	13.97	9.37	7.65
<i>Quercus m.</i>						10.17	6.23	4.03 ^a
<i>Tectona</i>							7.65	7.12
<i>Paulownia</i>								2.67 ^a
(d) Second derivative spectra; NIR range for selecting wavelengths: 800–1100 nm								
<i>Picea</i>	2.36 ^a	6.62	5.24 ^a	4.57 ^a	7.54	13.41	10.61	10.18
<i>Pseudotsuga</i>		4.54 ^a	2.93 ^a	5.71 ^a	6.29	12.41	8.29	8.23
<i>Cryptomeria</i>			2.18 ^a	7.75	3.61 ^a	9.13	4.57 ^a	3.91 ^a
<i>Cryptomeria</i> S.				7.64	5.32 ^a	11.18	5.39 ^a	5.94 ^a
<i>Fagus</i>					6.35	10.90	12.31	10.12
<i>Quercus m.</i>						6.19	7.28	3.96 ^a
<i>Tectona</i>							11.01	6.85
<i>Paulownia</i>								4.39 ^a

Cryptomeria: heartwood and sapwood; *Cryptomeria* S.: sapwood
NIR, near-infrared

^aThe distance was 6σ or less ($\sigma = 1$)

As S_{isd} decreases, each wood group is seen to be well separated. The S_{isd} for each analytical pattern is shown in Fig. 3. In each case, S_{isd} decreased as the number of selected wavelengths increased. It is known that the wavelengths in the second derivative spectra contributed more to the decrease in S_{isd} than that in the original spectra except for the following analytical pattern: a moisture content in the range from the air-dried to the fiber-saturated state and a wavelength from 800 to 1100 nm. When the wavelength was limited to the short range of 800–1100 nm, S_{isd} had a tendency to increase. When the three wavelengths were selected from the second derivative spectra, the discriminant analysis could be well performed independent of moisture conditions.

Results of discriminant analysis

Table 4 shows the final results of the discriminant analysis. For the discriminant analysis at 800–2500 nm, we had many correct results for the wood samples ranging from the air-dried to the fiber-saturated state. Especially, the wavelengths of 1720, 2232, and 2248 nm in the second derivative spectra resulted in completely correct results. The relations

between these second derivatives of absorbances for each wood species are displayed in Fig. 4. It is known that the woods in this group are well separated, which indicates that the spectra of the various wood species are sufficiently different at these three wavelengths. The wavelengths of 1720 and 2248 nm are assigned to the overtone of CH_3 stretching vibration and the combination of OH deformation and stretching vibration, respectively.¹ They are directly related to the wood components. When the wavelength for analysis was limited to the short range of 800–1100 nm, the percentage of correct results fell slightly. In this case, the wavelength derived from the absorption of water (around 980 nm) was often selected. Hence, there may be two bases for selecting the wavelength: (1) the chemical components of the wood and (2) the difference in moisture condition of the wood.

Such is true even for the samples ranging from the air-dried state to the fully saturated free water state. When the sample includes much free water inhomogeneously, the correct identification is less certain, whereas, the combination of three wavelengths at second derivative spectra (1415, 1672, and 2248 nm) resulted in high accuracy (98%). The relation between these second derivative absorbances for

Table 3. Mahalanobis' generalized distance between wood species with air-dried to fully saturated samples

Sample	<i>Pseudotsuga</i>	<i>Cryptomeria</i>	<i>Cryptomeria</i> S.	<i>Fagus</i>	<i>Quercus m.</i>	<i>Tectona</i>	<i>Paulownia</i>	<i>Quercus g.</i>
(a) Original spectra; NIR range for selecting wavelengths: 800–2500 nm								
<i>Picea</i>	3.69 ^a	7.77	5.83 ^a	27.43	12.49	10.76	14.14	17.79
<i>Pseudotsuga</i>		11.41	9.32	29.91	14.94	14.41	16.48	20.43
<i>Cryptomeria</i>			3.47 ^a	22.94	9.86	3.11 ^a	11.35	13.65
<i>Cryptomeria</i> S.				22.43	8.05	5.63 ^a	9.77	12.71
<i>Fagus</i>					15.02	20.94	13.42	9.88
<i>Quercus m.</i>						9.49	1.81 ^a	5.56
<i>Tectona</i>							10.73	12.11
<i>Paulownia</i>								4.43 ^a
(b) Second derivative spectra; NIR range for selecting wavelengths: 800–2500 nm								
<i>Picea</i>	3.85 ^a	3.51 ^a	5.43 ^a	23.73	14.38	7.65	15.21	15.51
<i>Pseudotsuga</i>		6.88	9.24	24.99	15.48	8.02	15.45	19.21
<i>Cryptomeria</i>			3.35 ^a	20.98	11.99	6.48	13.43	12.55
<i>Cryptomeria</i> S.				22.26	13.77	9.54	15.79	10.19
<i>Fagus</i>					9.57	17.06	10.46	20.52
<i>Quercus m.</i>						7.74	3.56 ^a	15.75
<i>Tectona</i>							7.75	16.43
<i>Paulownia</i>								19.09
(c) Original spectra; NIR range for selecting wavelengths: 800–1100 nm								
<i>Picea</i>	2.09 ^a	10.33	5.62 ^a	7.43	7.43	10.97	4.83 ^a	15.96
<i>Pseudotsuga</i>		12.21	6.13	6.15	7.34	12.31	4.61 ^a	17.59
<i>Cryptomeria</i>			12.22	16.18	14.11	10.21	12.47	12.16
<i>Cryptomeria</i> S.				5.77 ^a	2.66 ^a	7.43	3.01 ^a	12.81
<i>Fagus</i>					4.38 ^a	12.22	3.80 ^a	18.04
<i>Quercus m.</i>						8.17	3.06 ^a	13.83
<i>Tectona</i>							9.07	6.01
<i>Paulownia</i>								14.87
(d) Second derivative spectra; NIR range for selecting wavelengths: 800–1100 nm								
<i>Picea</i>	2.65 ^a	6.28	6.03	5.25 ^a	6.89	13.11	3.87 ^a	14.91
<i>Pseudotsuga</i>		3.65 ^a	5.11 ^a	5.94 ^a	4.97 ^a	10.52	4.31 ^a	13.04
<i>Cryptomeria</i>			6.31	8.62	4.53 ^a	7.25	7.11	11.47
<i>Cryptomeria</i> S.				4.66 ^a	2.59 ^a	9.92	3.57 ^a	9.24
<i>Fagus</i>					6.47	13.61	1.77 ^a	13.14
<i>Quercus m.</i>						7.41	5.26 ^a	6.11
<i>Tectona</i>							12.45	7.57
<i>Paulownia</i>								12.56

Cryptomeria: heartwood and sapwood. *Cryptomeria* S.: sapwood

^a The distance was 6σ or less

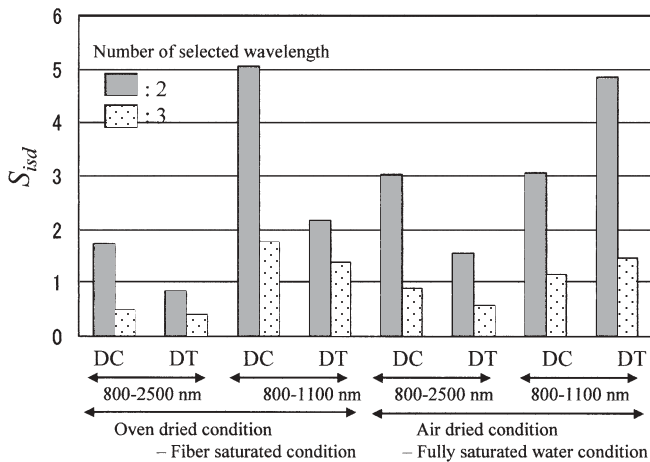


Fig. 3. Sum of inverse squared distances for various analytical patterns. DC, original spectra; DT, second derivative spectra; $S_{isd} = \sum (\frac{1}{d_i})^2$

each wood species are displayed in Fig. 5. A figure of 2248nm was also selected regardless of the moisture condition in a sample, so it may be the key wavelength for discriminant analysis.

Hence, the combination of NIRS and Mahalanobis' generalized distance provided superior ability to classify wood species. We must further examine the effect of the district in which the wood is grown and the lot of the wood samples for such classification, in terms of statistical "noise."

Conclusions

We examined methods for suitable discrimination of wood species without the influence of the moisture condition. The concept of Mahalanobis' generalized distance was applied to NIR spectra. In the discriminant analysis with second derivative spectra ranging from 800 to 2500nm, each wood group was well separated, and we had many correct results, where the selected wavelengths were often derived from the absorption of wood components. When the wavelengths for analysis were limited to the short range of 800–1100nm, the correct results diminished. In this case, the wavelength derived from the absorption of water (around 980nm) was often selected. Hence, there may be two bases for selecting the wavelength. The distances between softwoods were

Table 4. Results of discriminant analysis for wood species having various moisture conditions

Water condition in wood	Spectra	NIR range for selecting wavelengths (nm)	Selected wavelengths (nm)	Correct answer
Oven-dried state	Original	800–2500	2260, ^a 2300	90.9%
			2160, 2180, 2320	99.4%
Fiber saturated state	Second derivative	800–2500	2248, ^a 2264 ^a	96.4%
			1720, ^a 2232, 2248 ^a	100.0%
	Original	800–1100	948, 984 ^b	71.3%
			876, 1048, 1088 ^a	91.9%
	Second derivative	800–1100	1000, ^b 1096	86.8%
			976, ^b 1040, 1096	94.9%
Air-dried state	Original	800–2500	900, ^a 1120	81.6%
			1500, 2180, 2240 ^a	89.8%
Fully saturated free water state	Second derivative	800–2500	1752, 2280 ^a	83.7%
			1415, ^b 1672, ^a 2248 ^a	98.0%
	Original	800–1100	896, ^a 1028	83.7%
			888, 912, ^a 1100	89.8%
	Second derivative	800–1100	928, 992 ^b	65.3%
			856, 984, ^b 1048	91.8%

^a Wavelength derived from the absorption of wood components¹^b Wavelength derived from the absorption of water¹

Fig. 4. Relations between three second derivatives of absorbance. Water condition: oven-dried condition to fiber saturated condition. Wavelength: 800–2500 nm. Double circles, *Cryptomeria japonica* (heartwood and sapwood); filled circles, *Cryptomeria japonica* (sapwood); filled triangles, *Pseudotsuga menziesii*; open circles, *Picea sitchensis*; diamonds, *Tectona grandis*; crosses, *Quercus mongolica*; plus signs, *Paulownia tomentosa*; open triangles, *Quercus gilva*; inverted triangles, *Fagus crenata*

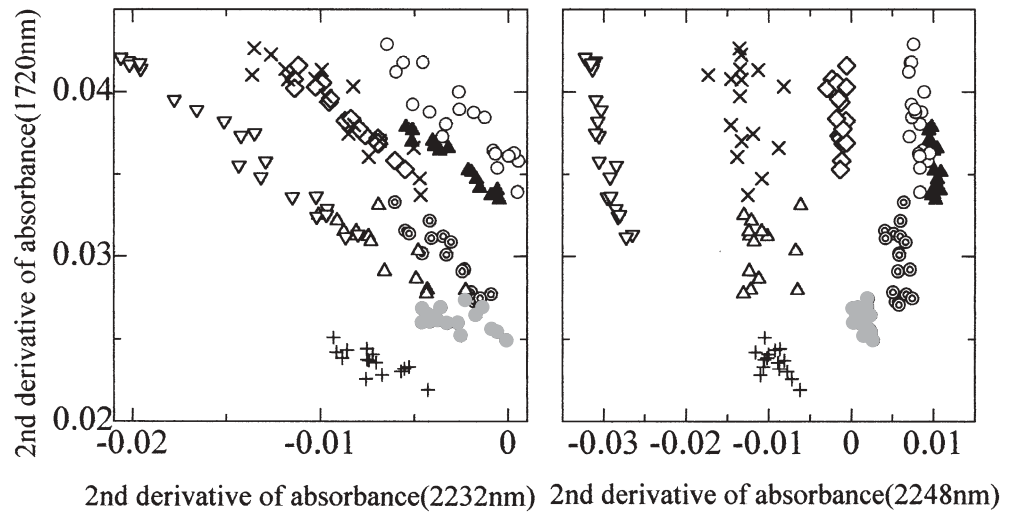
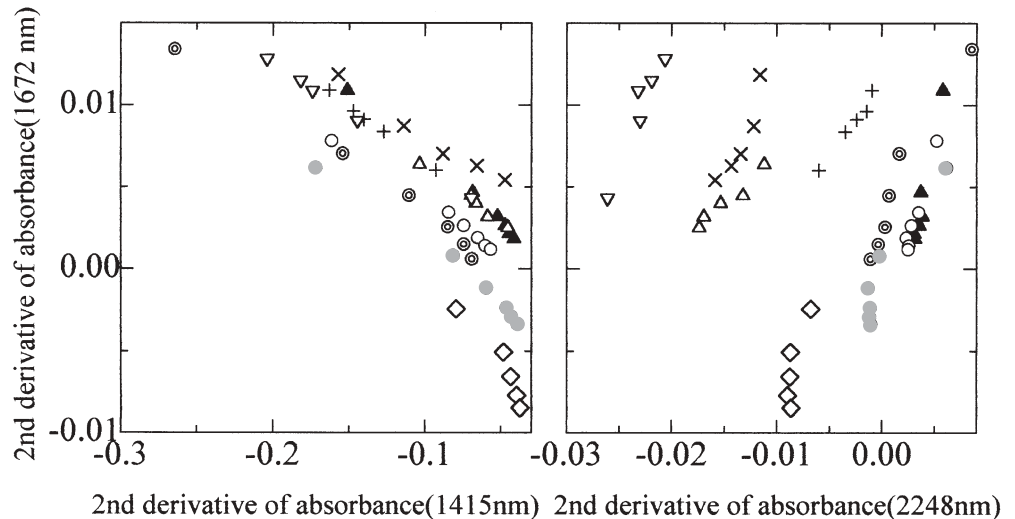


Fig. 5. Relations between three second derivatives of absorbance. Water condition: air-dried state to the fully saturated free water state. Wavelength: 800–2500 nm. Symbols are the same as in Fig. 4



relatively close independent of analytical pattern, so it was difficult to explain the difference in their spectroscopic characteristics. On the other hand, the distances between hardwoods were large, resulting in easy classification. The effect of lignin or extractives on the difference in NIR spectra of wood could explain the results. When a database of NIR spectra is properly constructed, which is the purpose of the analysis, effective discriminant analyses should be possible.

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